

Characterization of Eleven 2,5-Dimethoxy-N-(2-methoxybenzyl)-phenethylamine (NBOMe) Derivatives and Differentiation from their 3- and 4- Methoxybenzyl Analogues - Part II

Patrick A. Hays*, John F. Casale

U.S. Department of Justice
Drug Enforcement Administration
Special Testing and Research Laboratory
22624 Dulles Summit Court
Dulles, VA 20166-9509
[email address withheld at author's request]

ABSTRACT: The characterization of the 33 2,5-dimethoxy-N-(2-methoxybenzyl)-, (3-methoxybenzyl)-, and (4-methoxybenzyl) phenethylamine (NBOMe) derivatives via NMR spectroscopy is presented. The data enables differentiation of all 33 compounds.

KEYWORDS: Hallucinogens, NBOMe, 25H-NBOMe, 25B-NBOMe, 25C-NBOMe, 25D-NBOMe, 25E-NBOMe, 25I-NBOMe, 25N-NBOMe, 25P-NBOMe, 25T2-NBOMe, 25T4-NBOMe, 25T7-NBOMe, NMR, Designer Drugs, Synthesis, Characterization, Forensic Chemistry, Positional Isomers.

Introduction

Part I of this study presented the Fourier transform infrared and mass spectral data for the series of designer drugs commonly referred to as "NBOMe" compounds (1). Herein we present the NMR spectra (proton and carbon-13) for both the HCl salt and the free base for each of the three methoxybenzyl positional isomers for all 11 specified NBOMe compounds (Figure 1).

Experimental

Chemicals

Deuterated chloroform (CDCl_3) containing 0.05% v/v tetramethylsilane (TMS, 0 ppm reference) and deuterium oxide (D_2O) were both purchased from Cambridge Isotope Laboratories, Inc. (Tewksbury, MA). Sodium bicarbonate and anhydrous sodium sulfate were purchased from Sigma-Aldrich (St. Louis, MO). All 33 NBOMe HCl samples were synthesized at this laboratory.

Nuclear Magnetic Resonance Spectroscopy

All NMR spectra were obtained using the

following instruments: Mercury 400 MHz NMR with a 5 mm Nalorac Pulsetune indirect detection probe; a 400MR with a 5 mm Protune Indirect Detection probe; a 400MR-DD2 with a 5 mm OneNMR Probe; or a VNMRs 600 MHz NMR with a 5 mm broadband probe (all from Agilent, Palo Alto, CA). All probes used pulse field gradients. The sample temperature was maintained at 25°C. Standard Agilent pulse sequences were used to collect the following spectra: Proton, carbon-13 (proton decoupled), and gradient versions of the 2-Dimensional experiments HSQC and HMBC. The HCl salt of each compound was dissolved in CDCl_3 and the spectra acquired. The corresponding free base of each HCl salt was then formed by basifying the respective solution with saturated sodium bicarbonate in D_2O ; the isolated CDCl_3 solution was then dried with anhydrous sodium sulfate, and the spectra acquired. Data processing and structure elucidation were performed using Structure Elucidator software from Applied Chemistry Development (ACD/Labs, Toronto, Canada).

Results and Discussion

The HCl salt and the free base of every NBOMe derivative were soluble in CDCl_3 . The proton spectrum contains three basic regions of interest (see Figure 2): a) The NH region (9-10 ppm) which integrates to 2 for the HCl salt (but no signal after D_2O -sodium bicarbonate extraction); b) the aromatic region (6.5-7.5 ppm) containing the signals for the six NBOMe benzene protons (seven for 25H-NBOMe); and c) the aliphatic region (2.9-4.5 ppm) which contains the three methoxy singlets and signals for the bridging $\text{CH}_2\text{-N-CH}_2\text{-CH}_2$ protons. The carbon-13 spectrum (see Figure 3) is divided into five basic regions of interest: a) The three aromatic carbons bonded to oxygen (145-160 ppm); b) the other nine aromatic carbons (100-135 ppm, with the exception of 25I-NBOMe having one carbon at 80-85 ppm for the carbon bonded to iodine); c) the three methoxy carbons (about 55 ppm); d) the $\text{CH}_2\text{-CH}_2$ group bonded to nitrogen (about 45 ppm); and e) the last CH_2 bonded to the phenyl group (about 25 ppm). The proton spectrum definitively determines the position of the benzyl methoxy group as *ortho*, *meta*, or *para*. When correlated with the molecular weight and other NMR data, the specific NBOMe compound can be unambiguously identified.

Tables I-III present the proton NMR assignments for all 33 compounds as the HCl salts, while Tables IV-VI are the assignments for the same compounds as their corresponding free bases. Tables VII-IX present the carbon-13 NMR assignments for all 33 compounds as the HCl salts, while Tables X-XII are the assignments for the same compounds as their corresponding free bases. Each Table contains the 11 NBOMe compounds with the benzyl methoxy substituent in the same position (i.e., the NBOMe HCl compounds with the methoxy benzyl in the *ortho* position are in Table I for proton and Table VII for carbon-13, while the *meta* substituted compounds are in Tables II and VIII, and so on).

Proton Spectra

Common to all NBOMe compound proton spectra are the peaks in the aromatic region (6.5-7.5 ppm)

with its six protons (four benzyl and two *para*-phenyl singlets, with the exception of 25H-NBOMe, which has seven); the methoxy region (3.6-4.2 ppm) with its three methoxy singlets and the benzyl CH_2 triplet (HCl spectra) or singlet (base spectra); and the ethylene region 2.7-3.2 ppm with its multiplets. Additional peaks, if present, can aid in the identification of a substituent at the 4-phenyl position, if that substituent also contains one or more protons.

The aromatic region may be used to determine whether the methoxy position on the benzyl ring is *ortho*, *meta*, or *para*, since the coupling constants for an aromatic proton change based on whether another proton it is coupled to is *alpha* (7-8 Hz coupling) or *beta* (1-3 Hz) on the ring. Using only couplings >5 Hz to describe the proton peak pattern, NB2OMe spectra contain two doublets and two triplets; NB3OMe spectra contain one broadened singlet (actually a doublet of doublets with small couplings), two doublets, and one triplet; and NB4OMe spectra have two doublets, each representing two hydrogens. In looking more closely at the coupling constants of some triplets, it is evident that they are actually doublets of doublets whose coupling constants are similar (e.g., 7 and 8 Hz). To illustrate the differences, Figure 4 shows the aromatic region of the proton spectra of the three positional isomers of 25I-NBOMe HCl dissolved in CDCl_3 . The smaller coupling constants are due to *meta* coupling (4 bonds) and range from ~0.9 Hz to ~2.5 Hz. In 25I-NB3OMe HCl (Figure 4B), the 7.20 ppm doublet of doublets (which looks like a small triplet) represents H-2 with couplings to H-4 (~2.5 Hz) and H-6 (~1 Hz). In addition to the aromatic benzyl protons, all NBOMe proton spectra, except 25H-NBOMe, will have two singlets in the aromatic region, which are caused by the phenyl protons on C-3 and C-6 (they are *para* to each other and have no discernable coupling). For 25H-NBOMe, the substituent at C-4 is hydrogen, and the aromatic region will therefore show seven (not six) hydrogens, and the phenyl proton pattern will be a doublet (~8 Hz), doublet of doublets (~8, ~2 Hz), and doublet (~2 Hz), characteristic of a 2,5-disubstituted phenyl ring.

The aliphatic region is less helpful in differentiating positional isomers of NBOMe, but is still useful in identification (Figure 5). There are three tall methoxy singlets between 3.6-3.85 ppm; the benzyl CH₂ triplet (HCl) between 3.9-4.2 ppm or singlet (base) between 3.7-3.8 ppm; and the CH₂-CH₂ multiplets between 2.9-3.2 ppm. Of note in this region is the fact that the benzyl CH₂ triplet chemical shift in HCl spectra is highest in the NB2OMe spectrum, followed by the NB3OMe spectrum, and then by the NB4OMe spectrum.

If the substituent is unknown then the following procedure should help in identifying it:

1. Determine the molecular weight by high resolution mass spectrometry to derive the molecular formula. If high resolution mass spectrometry is not available, then take the molecular ion and subtract it from 300 (i.e., the nominal mass for C₁₈H₂₂NO₃). Some example remainders are: 1 = hydrogen, 15 = methyl, 35 = chlorine, 79 = bromine, and 127 = iodine. Standard mass spectra can help identify many substituents, especially the halogens.

2. Determine how many hydrogens are present in the molecule from the proton NMR spectrum (not counting the broad singlet near 9 ppm) and subtract this number from 21. Note the location of any *extra* hydrogens in the proton spectrum (i.e., chemical shift, number, and peak pattern); these are on the substituent.

- a. If there are no extra hydrogens, then the extra molecular weight will be from a substituent that has no hydrogens (e.g., -NO₂).

- b. If there are extra hydrogens, use their peak pattern and chemical shift, to help determine the substituent's identity.

3. Determine the number of carbons from the carbon-13 NMR spectrum and subtract from 18 for NB2OMe and NB3OMe, or from 16 for NB4OMe (the latter compounds have *para* substitution on the benzyl group, so the *ortho* and *meta* carbons are equivalent, and produce only two peaks for four carbons).

Carbon Spectra

The NB2OMe and NB3OMe carbon-13 spectra contain 12 aromatic peaks, while the NB4OMe carbon-13 spectra contain 10 aromatic peaks due to symmetry of the *para*-methoxyphenyl. The aliphatic portion of the NBOMe spectra contains three methoxy and three methylene carbon-13 peaks. For the HCl salts, the CH₂-CH₂-N carbons have chemical shifts of about 28 and 45 ppm, while the benzyl CH₂ is between 45-50 ppm. The NB2OMe HCl salts have their benzyl CH₂ at 46-47 ppm, while the NB3OMe HCl and NB4OMe HCl benzyl CH₂ are at ~50 ppm. Similarly, the NBOMe base compounds' CH₂-CH₂ chemical shifts are at ~31 and ~49 ppm, while the benzyl CH₂ is found at ~49 ppm (NB2OMe) or ~53 ppm (NB3OMe and NB4OMe). 25I-NBOMe compounds (HCl and base) have a distinctive aromatic carbon, bonded to iodine, at 82-84 ppm.

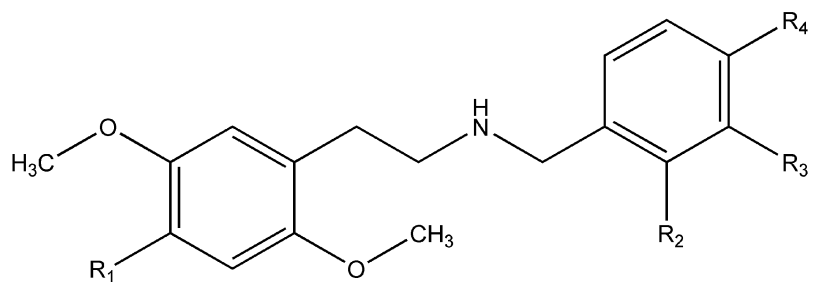
Conclusions

All of the 2,5-dimethoxy-N-(2-methoxybenzyl) phenethylamines analyzed in this study are distinguishable from their 3- and 4-methoxybenzyl analogues via proton and carbon-13 NMR spectroscopy. A quick determination of whether an NBOMe compound is the 2-, 3-, or 4-methoxybenzyl substituted form is easily accomplished by inspection of the aromatic region of its proton NMR. In addition, a simple stepwise approach can help determine the identity of a substituent at the 4-phenyl position, using the NMR spectra and the molecular weight derived from mass spectrometry.

Reference

1. Casale JF, Hays PA. Characterization of eleven 2,5-dimethoxy-N-(2-methoxybenzyl) phenethylamine (NBOMe) derivatives and differentiation from their 3- and 4-methoxy-benzyl analogues - Part I. Microgram Journal 2012;9(2):84-109.

Figure 1. Structural formulas.



Compound	R ₁	R ₂	R ₃	R ₄
25H-NB2OMe (1)	H	OCH ₃	H	H
25H-NB3OMe (2)	H	H	OCH ₃	H
25H-NB4OMe (3)	H	H	H	OCH ₃
25B-NB2OMe (4)	Br	OCH ₃	H	H
25B-NB3OMe (5)	Br	H	OCH ₃	H
25B-NB4OMe (6)	Br	H	H	OCH ₃
25C-NB2OMe (7)	Cl	OCH ₃	H	H
25C-NB3OMe (8)	Cl	H	OCH ₃	H
25C-NB4OMe (9)	Cl	H	H	OCH ₃
25D-NB2OMe (10)	CH ₃	OCH ₃	H	H
25D-NB3OMe (11)	CH ₃	H	OCH ₃	H
25D-NB4OMe (12)	CH ₃	H	H	OCH ₃
25E-NB2OMe (13)	C ₂ H ₅	OCH ₃	H	H
25E-NB3OMe (14)	C ₂ H ₅	H	OCH ₃	H
25E-NB4OMe (15)	C ₂ H ₅	H	H	OCH ₃
25I-NB2OMe (16)	I	OCH ₃	H	H
25I-NB3OMe (17)	I	H	OCH ₃	H
25I-NB4OMe (18)	I	H	H	OCH ₃
25N-NB2OMe (19)	NO ₂	OCH ₃	H	H
25N-NB3OMe (20)	NO ₂	H	OCH ₃	H
25N-NB4OMe (21)	NO ₂	H	H	OCH ₃
25P-NB2OMe (22)	CH ₂ CH ₂ CH ₃	OCH ₃	H	H
25P-NB3OMe (23)	CH ₂ CH ₂ CH ₃	H	OCH ₃	H
25P-NB4OMe (24)	CH ₂ CH ₂ CH ₃	H	H	OCH ₃
25T2-NB2OMe (25)	CH ₃ CH ₂ S	OCH ₃	H	H
25T2-NB3OMe (26)	CH ₃ CH ₂ S	H	OCH ₃	H
25T2-NB4OMe (27)	CH ₃ CH ₂ S	H	H	OCH ₃
25T4-NB2OMe (28)	(CH ₃) ₂ CHS	OCH ₃	H	H
25T4-NB3OMe (29)	(CH ₃) ₂ CHS	H	OCH ₃	H
25T4-NB4OMe (30)	(CH ₃) ₂ CHS	H	H	OCH ₃
25T7-NB2OMe (31)	CH ₃ (CH ₂) ₂ S	OCH ₃	H	H
25T7-NB3OMe (32)	CH ₃ (CH ₂) ₂ S	H	OCH ₃	H
25T7-NB4OMe (33)	CH ₃ (CH ₂) ₂ S	H	H	OCH ₃

Figure 2. Proton spectrum of 25C-NB2OMe HCl in CDCl₃ with assignments. The two singlets at 6.8 and 6.9 ppm (a) are protons on the phenyl group which are *para* to each other; the proton at 4.1 ppm (b) is a triplet due to coupling with the NH₂⁺; the tall singlets at 3.5-3.8 ppm (c) are the methoxy groups; and the multiplet at 3.1 ppm (d) is the bridging ethyl group.

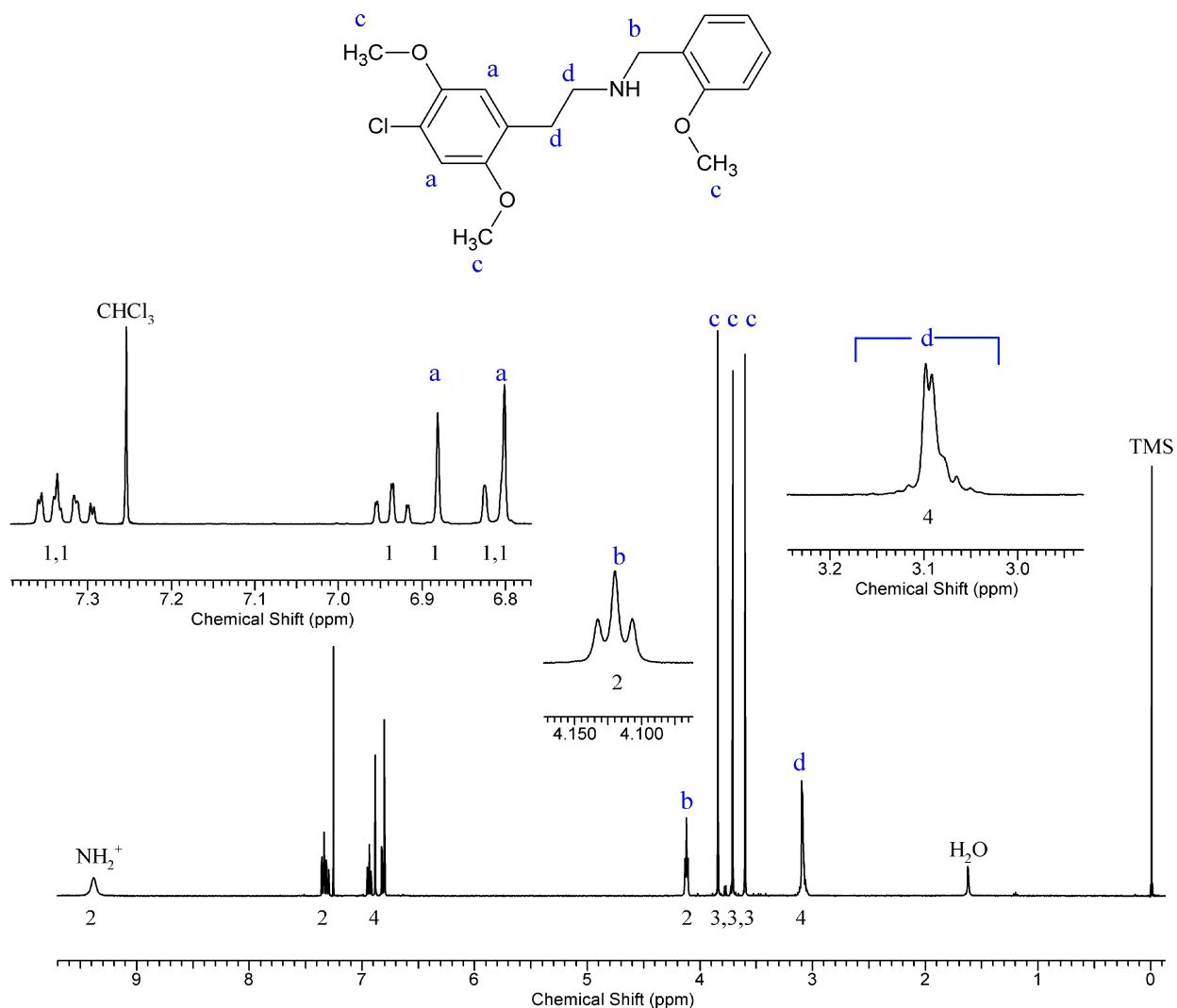


Figure 3. Carbon-13 spectrum of 25C-NB2OMe HCl in CDCl₃. Aromatic carbons bonded to oxygen are at 149-158 ppm; nine remaining benzene carbons are at 110-132 ppm; methoxy carbons are at 55-57 ppm; and bridging methylenes are at 28, 45, and 47 ppm.

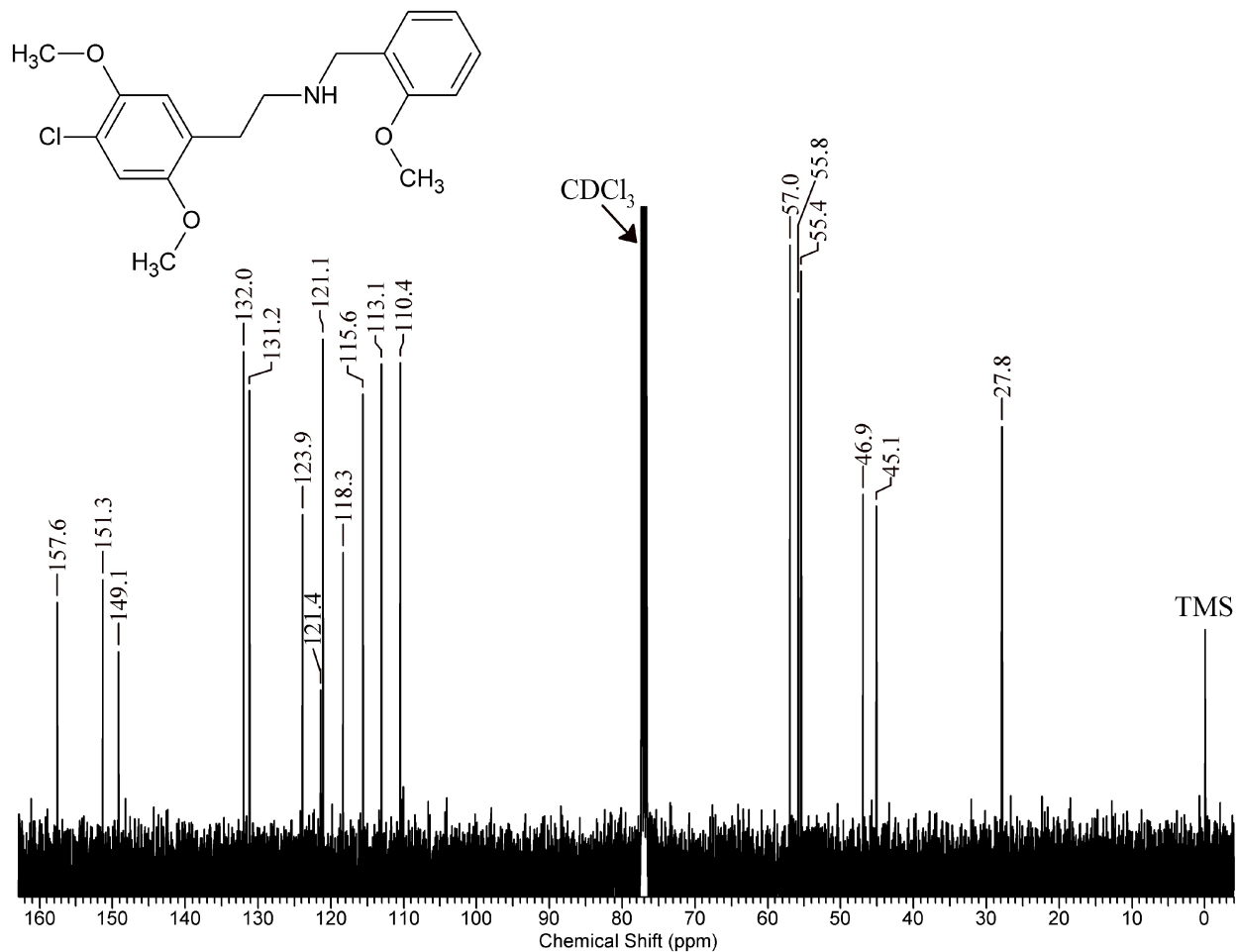


Figure 4. Proton NMR spectra of aromatic region of 25I-NBOMe HCl dissolved in CDCl_3 ; with the benzyl methoxy at the *ortho* (A), *meta* (B), and *para* (C) positions. *Ortho* substitution (A) is easily detected by its two apparent doublets and two apparent triplets. *Meta* substitution (B) yields one triplet, one doublet, one doublet of doublets, and one small coupling doublet of doublets (7.20 ppm). *Para* substitution (C) is demonstrated by its two doublets which contain 2 hydrogens each. The two singlets at 6.7 and 7.1 ppm are the phenyl protons at C-6 and C-3, respectively.

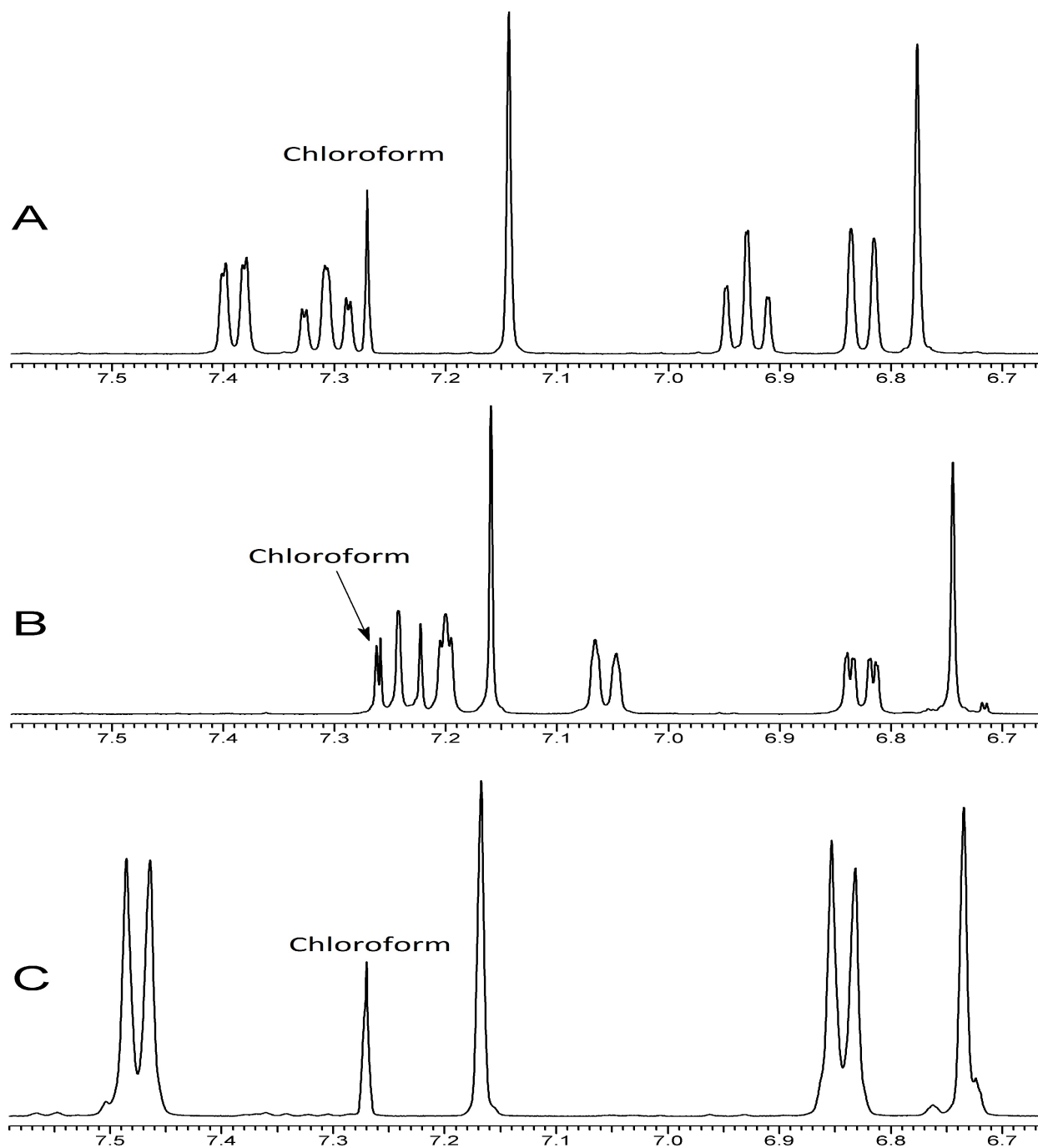


Figure 5. Proton spectra of aliphatic region of 25I-NBOMe HCl dissolved in CDCl_3 ; with the benzyl methoxy at the *ortho* (A), *meta* (B), and *para* (C) positions. The three methoxy groups are the tall singlets between 3.6-3.85 ppm; while the benzyl CH_2 is the triplet between 3.9-4.2 ppm, and the $\text{CH}_2\text{-CH}_2$ bridging group are the multiplets between 2.9-3.2 ppm.

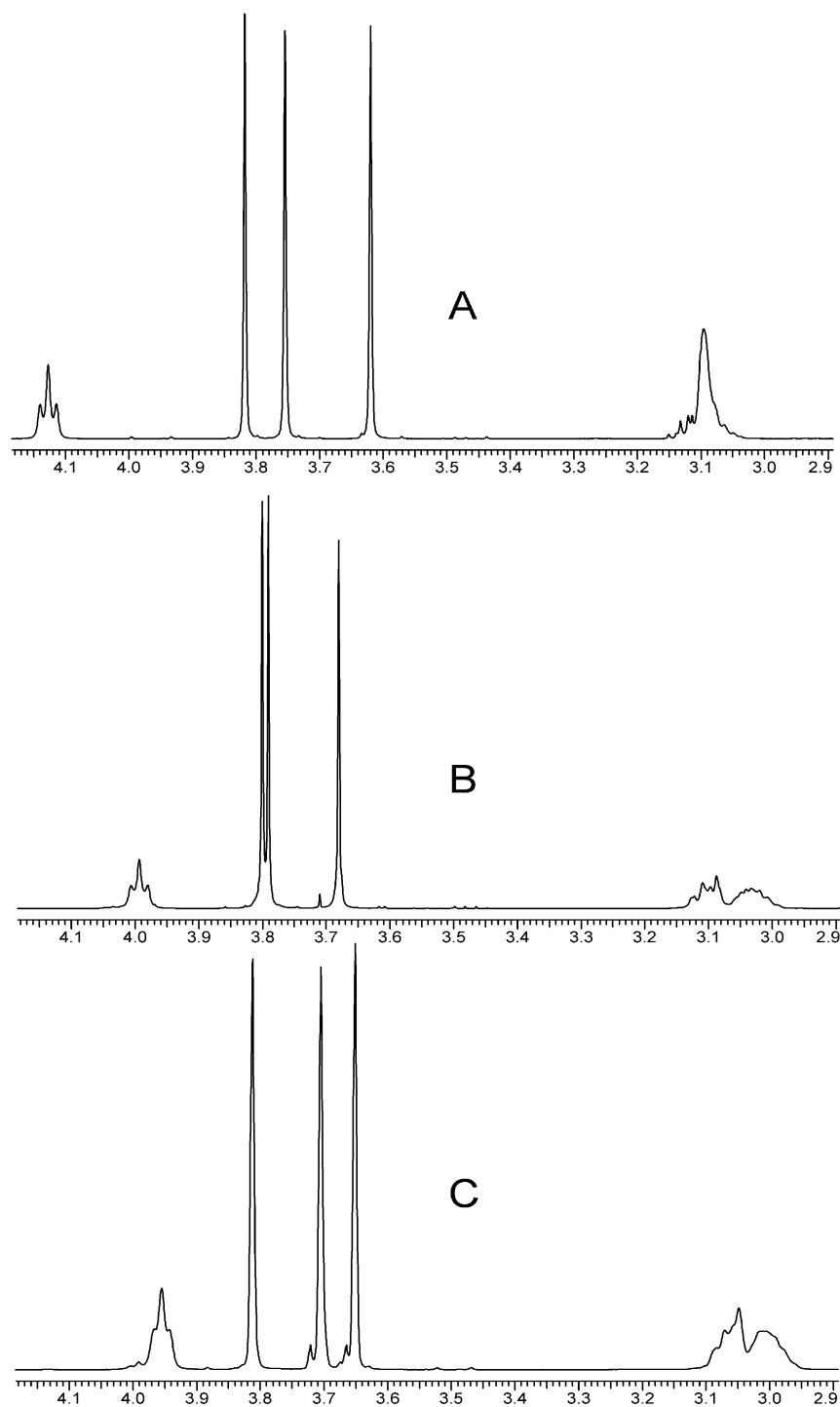


Table I. Proton NMR Assignments *ortho*-Methoxyphenyl NBOMe HCl Compounds.

	25H-NB2OMe HCl (600 MHz)		25D-NB2OMe HCl		25E-NB2OMe HCl		25P-NB2OMe HCl	
position	ppm	peak multiplicity	ppm	peak multiplicity	ppm	peak multiplicity	ppm	peak multiplicity
benzyl 3	6.82	bd(8.2)	6.80	bd(8.3)	6.80	bd(8.3)	6.80	bd(8.0)
4	7.31	ddd(8.2, 7.8, 1.3)[atd]	7.32	ddd(8.3, 7.7, 1.5)[atd]	7.30	ddd(8.3, 7.5, 1.6)[atd]	7.31	ddd(8.0, 7.6, 1.6)
5	6.94	bt(7.8)	6.94	ddd(7.7, 7.4, 0.9)[atd]	6.94	ddd(7.6, 7.5, 0.8)[atd]	6.94	ddd(7.6, 7.4, 0.9)
6	7.4	dd(7.8, 1.3)	7.36	dd(7.4, 1.5)	7.39	dd(7.6, 1.6)	7.38	dd(7.4, 1.6)
location of methoxy	2		2		2		2	
OCH3	3.74	s	3.67	s	3.70	s	3.70	s
CH2NHCH2CH2-Ph	4.17	t(5.2)	4.15	t(5.2)	4.16	t(5.1)	4.15	t(5.1)
CH2NH CH2CH2-Ph	3.11	m	3.09	m	3.10	m	3.10	m
CH2NHCH2 CH2-Ph	3.11	m	3.09	m	3.10	m	3.10	m
Phenyl 3	6.71	d(8.8)	6.60	s	6.62	s	6.59	s
4	6.74	dd(8.8, 2.8)	0.00		0.00		0.00	
6	6.77	d(2.8)	6.70	s	6.71	s	6.71	s
2-OCH3	3.63	s	3.60	s	3.62	s	3.62	s
5-OCH3	3.73	s	3.76	s	3.75	s	3.74	s
NH2+	9.43	vbs	9.33	vbs	9.40	vbs	9.37	vbs
4-substituent	H		CH3		CH2-CH3		propyl	
			2.18	s	2.57	q(7.6)	2.52	dd(8.6, 6.8)
					1.15	t(7.6)	1.56	dqd(8.6, 7.3, 6.8)
							0.94	t(7.3)
	25N-NB2OMe HCl		25C-NB2OMe HCl		25B-NB2OMe HCl		25I-NB2OMe HCl	
benzyl 3	6.85	d(8.4)	6.82	bd(~7.5)	6.82	bd(8.0)	6.83	bd(8.3)
4	7.29	dd(~8.4, ~7.4)	7.32	m	7.31	ddd(8.0, 7.8, 1.6)	7.31	ddd(8.3, 7.8, 1.5)
5	6.92	t(~7.4)	6.94	td(7.4, 0.9)	6.93	ddd(7.8, 7.5, 1.6)	6.93	bdd(7.8, 7.2)
6	7.42	d(7.6)	7.35	m	7.38	dd(7.5, 1.6)	7.39	dd(7.7, 1.3)
location of methoxy	2		2		2		2	
OCH3	3.85	s	3.72	s	3.74	s	3.75	s
CH2NHCH2CH2-Ph	4.10	t(5.1)	4.13	t(5.2)	4.13	t(5.0)	4.12	t(5.1)
CH2NH CH2CH2-Ph	3.10	m	3.09	m	3.09	m	3.10	m
CH2NHCH2 CH2-Ph	3.20	m	3.10	m	3.09	m	3.10	m
Phenyl 3	7.31	s	6.81	s	6.96	s	7.14	s
4								
6	7.13	s	6.89	s	6.87	s	6.78	s
2-OCH3	3.73	s	3.61	s	3.62	s	3.61	s
5-OCH3	3.94	s	3.85	s	3.84	s	3.82	s
NH2+	9.65	vbs	9.39	vbs	9.43	vbs	9.47	vbs
4-substituent	NO2		Cl		Br		I	
	25T2-NB2OMe HCl		25T4-NB2OMe HCl		25T7-NB2OMe HCl			
benzyl 3	6.82	bd(8.2)	6.83	bd(7.7)	6.82	bd(8.5)		
4	7.30	ddd(8.2, 7.6, 1.7)	7.30	ddd(8.1, 7.7, 1.7)	7.31	td(7.4, 0.8)		
5	6.93	ddd(7.6, 7.5, 0.8)	6.93	ddd(8.1, 7.7, 0.9)	6.93	ddd(8.5, 7.4, 1.5)		
6	7.41	dd(7.5, 1.7)	7.40	dd(7.7, 1.7)	7.39	dd(7.4, 1.5)		
location of methoxy	2		2		2			
OCH3	3.76	s	3.76	s	3.74	s		
CH2NHCH2CH2-Ph	4.15	t(5.2)	4.15	t(5.2)	4.14	t(5.2)		
CH2NH CH2CH2-Ph	3.11	m	3.11	m	3.08	m		
CH2NHCH2 CH2-Ph	3.11	m	3.12	m	3.12	m		
Phenyl 3	6.74	s	6.83	s	6.74	s		
4								
6	6.77	s	6.79	s	6.76	s		
2-OCH3	3.82	s	3.64	s	3.64	s		
5-OCH3	3.65	s	3.82	s	3.83	s		
NH2+	9.44	vbs	9.44	vbs	9.44	vbs		
4-substituent	S-CH2CH3		S-CH(CH3)2		S-CH2CH2CH3			
	2.90	q(7.3)	3.47	septet(6.7)	2.84	dd(~7.5, ~7.0)		
	1.29	t(7.3)	1.26	d(6.7)	1.66	sextet(7.3)		
					1.03	t(7.3)		

Abbreviations: a – apparent, b – broad, d – doublet, m – multiplet, q – quartet, s – singlet, t – triplet, vbs – very broad singlet

Table II. Proton NMR Assignments *meta*-Methoxyphenyl NBOMe HCl Compounds.

	25H-NB3OMe HCl		25D-NB3OMe HCl		25E-NB3OMe HCl		25P-NB3OMe HCl	
position	ppm	peak multiplicity	ppm	peak multiplicity	ppm	peak multiplicity	ppm	peak multiplicity
benzyl 2	7.26	m	7.23	m	7.23	m	7.23	m
4	6.84	dd(8.4, 2.5)	6.84	ddd(8.3, 2.6, <1)	6.83	dd(8.1, 2.2)	6.83	dd(8.4, 2.5)
5	7.26	m	7.25	m	7.24	m	7.23	m
6	7.08	bd(7.6)	7.07	bd(7.7)	7.07	bd(7.4)	7.07	bd(7.6)
location of methoxy	3		3		3		3	
OCH3	3.81	s	3.80	s	3.80	s	3.80	s
CH2NHCH2CH2-Ph	4.06	t(5.1)	4.03	t(5.2)	4.03	t(5.1)	4.03	t(5.2)
CH2NH CH2CH2-Ph	3.05	m	3.05	m	3.05	m	3.05	m
CH2NHCH2 CH2-Ph	3.15	m	3.13	m	3.13	m	3.13	m
Phenyl 3	6.72	m	6.61	s	6.62	s	6.60	s
4	6.72	m						
6	6.78	m	6.70	s	6.71	s	6.71	s
2-OCH3	3.68	s	3.67	s	3.69	s	3.68	s
5-OCH3	3.72	s	3.75	s	3.74	s	3.73	s
NH2+	10.04	vbs	9.97	vbs	10.00	vbs	10.00	vbs
4-substituent	H		CH3		CH2-CH3		propyl	
			2.17	s	2.57	q(7.5)	2.52	dd(~8, ~7)
					1.15	t(7.5)	1.56	a-sextet(7.3)
							0.93	t(7.3)
	25N-NB3OMe HCl		25C-NB3OMe HCl		25B-NB3OMe HCl		25I-NB3OMe HCl	
benzyl 2	7.20	dd(2.5, 1.2)	7.21	dd(2.5, 1.3)	7.21	dd(2.5, 1.3)	7.20	dd(2.5, 0.9)
4	6.82	ddd(8.4, 2.5, <1)	6.83	dd(8.2, 2.5)	6.83	ddd(8.0, 2.5, 1.3)	6.83	ddd(8.4, 2.5, <1)
5	7.24	dd(8.4, 7.4)	7.25	dd(8.2, 7.5)	7.25	dd(8.0, 7.6)	7.25	dd(8.4, 7.6)
6	7.07	bd(7.4)	7.07	bd(7.5)	7.07	bd(7.6)	7.06	bd(7.6)
location of methoxy	3		3		3		3	
OCH3	3.79	s	3.79	s	3.79	s	3.80	s
CH2NHCH2CH2-Ph	4.00	t(5.0)	4.01	t(5.1)	4.01	t(5.2)	4.00	t(5.2)
CH2NH CH2CH2-Ph	3.08	m	3.04	m	3.04	m	3.03	m
CH2NHCH2 CH2-Ph	3.19	m	3.12	m	3.11	m	3.11	m
Phenyl 3	7.34	s	6.83	s	6.98	s	7.16	s
4								
6	7.08	s	6.87	s	6.84	s	6.75	s
2-OCH3	3.77	s	3.69	s	3.69	s	3.69	s
5-OCH3	3.92	s	3.83	s	3.82	s	3.81	s
NH2+	10.02	vbs	9.96	vbs	10.00	vbs	10.00	vbs
4-substituent	NO2		Cl		Br		I	
	25T2-NB3OMe HCl		25T4-NB3OMe HCl		25T7-NB3OMe HCl			
benzyl 2	7.22	m	7.23	d(2.3)	7.22	m		
4	6.83	ddd(7.3, 2.4, 0.9)	6.83	dd(7.6, 2.3)	6.84	bdd(8.3, 2.3)		
5	7.25	t(~7.4)	7.25	t(7.6)	7.25	dd(8.3, 7.7)		
6	7.07	bd(7.6)	7.07	bd(7.6)	7.07	bd(7.6)		
location of methoxy	3		3		3			
OCH3	3.80	s	3.80	s	3.80	s		
CH2NHCH2CH2-Ph	4.03	t(5.3)	4.02	t(5.1)	4.02	t(5.2)		
CH2NH CH2CH2-Ph	3.05	m	3.06	m	3.04	m		
CH2NHCH2 CH2-Ph	3.13	m	3.14	m	3.13	m		
Phenyl 3	6.77	s	6.84	s	6.76	s		
4								
6	6.76	s	6.77	s	6.75	s		
2-OCH3	3.70	s	3.70	s	3.70	s		
5-OCH3	3.82	s	3.81	s	3.82	s		
NH2+	9.96	vbs	9.99	vbs	10.00	vbs		
4-substituent	S-CH2CH3		S-CH(CH3)2		S-CH2CH2CH3			
	2.88	q(7.4)	3.46	septet(6.8)	2.83	dd(~7.4, ~7.1)		
	1.28	t(7.4)	1.25	d(6.8)	1.64	sextet(7.3)		
					1.01	t(7.3)		
Abbreviations: a – apparent, b – broad, d – doublet, m – multiplet, q – quartet, s – singlet, t – triplet, vbs – very broad singlet								

Table III. Proton NMR Assignments *para*-Methoxyphenyl NBOMe HCl Compounds.

	25H-NB4OMe HCl		25D-NB4OMe HCl		25E-NB4OMe HCl		25P-NB4OMe HCl	
position	ppm	peak multiplicity	ppm	peak multiplicity	ppm	peak multiplicity	ppm	peak multiplicity
benzyl 2	7.50	d(8.7)	7.48	d(8.7)	7.48	d(8.7)	7.48	d(8.6)
3	6.86	d(8.7)	6.85	d(8.7)	6.85	d(8.7)	6.85	d(8.6)
5	6.86	d(8.7)	6.85	d(8.7)	6.85	d(8.7)	6.85	d(8.6)
6	7.50	d(8.7)	7.48	d(8.7)	7.48	d(8.7)	7.48	d(8.6)
location of methoxy	4		4		4		4	
OCH3	3.70	s	3.67	s	3.67	s	3.67	s
CH2NHCH2CH2-Ph	4.00	t(5.3)	3.98	t(5.0)	3.99	t(5.3)	3.98	t(5.1)
CH2NH CH2CH2-Ph	3.03	m	3.01	m	3.03	m	3.02	m
CH2NHCH2 CH2-Ph	3.11	m	3.11	m	3.09	m	3.08	m
Phenyl 3	6.72	d(1.6)[2nd order effects]	6.62	s	6.63	s	6.60	s
4	6.72	d(1.6)[2nd order effects]						
6	6.77	t(1.6)	6.69	s	6.70	s	6.70	s
2-OCH3	3.68	s	3.69	s	3.71	s	3.70	s
5-OCH3	3.72	s	3.75	s	3.75	s	3.74	s
NH2+	9.91	vbs	9.84	vbs	9.84	vbs	9.85	vbs
4-substituent	H		CH3		CH2CH3		propyl	
			2.17	s	2.58	q(7.5)	2.52	dd(~8,~7.3)
					1.16	t(7.5)	1.56	a-sextet(7.3)
							0.93	t(7.3)
	25N-NB4OMe HCl		25C-NB4OMe HCl		25B-NB4OMe HCl		25I-NB4OMe HCl	
benzyl 2	7.47	d(8.7)	7.48	d(8.6)	7.47	d(8.7)	7.47	d(8.5)
3	6.84	d(8.7)	6.85	d(8.6)	6.84	d(8.7)	6.84	d(8.5)
5	6.84	d(8.7)	6.85	d(8.6)	6.84	d(8.7)	6.84	d(8.5)
6	7.47	d(8.7)	7.48	d(8.6)	7.47	d(8.7)	7.47	d(8.5)
location of methoxy	4		4		4		4	
OCH3	3.65	s	3.66	s	3.65	s	3.65	s
CH2NHCH2CH2-Ph	3.94	(under OCH3 singlet)	3.95	t(5.2)	3.95	t(5.1)	3.95	t(5.0)
CH2NH CH2CH2-Ph	3.04	m	3.01	m	3.00	m	3.00	m
CH2NHCH2 CH2-Ph	3.13	m	3.07	m	3.06	m	3.07	m
Phenyl 3	7.35	s	6.83	s	6.98	s	7.17	s
4								
6	7.06	s	6.85	s	6.82	s	6.73	s
2-OCH3	3.79	s	3.71	s	3.71	s	3.70	s
5-OCH3	3.94	s	3.84	s	3.83	s	3.81	s
NH2+	9.92	vbs	9.92	vbs	9.89	vbs	9.91	vbs
4-substituent	NO2		Cl		Br		I	
	25T2-NB4OMe HCl		25T4-NB4OMe HCl		25T7-NB4OMe HCl			
benzyl 2	7.49	d(8.6)	7.49	d(8.6)	7.48	d(8.7)		
3	6.85	d(8.6)	6.85	d(8.6)	6.85	d(8.7)		
5	6.85	d(8.6)	6.85	d(8.6)	6.85	d(8.7)		
6	7.49	d(8.6)	7.49	d(8.6)	7.48	d(8.7)		
location of methoxy	4		4		4			
OCH3	3.66	s	3.66	s	3.66	s		
CH2NHCH2CH2-Ph	3.97	t(5.2)	3.97	t(5.3)	3.97	t(5.1)		
CH2NH CH2CH2-Ph	3.01	m	3.03	m	3.02	m		
CH2NHCH2 CH2-Ph	3.09	m	3.10	m	3.09	m		
Phenyl 3	6.77	s	6.85	s	6.76	s		
4								
6	6.75	s	6.76	s	6.74	s		
2-OCH3	3.72	s	3.71	s	3.72	s		
5-OCH3	3.83	s	3.82	s	3.83	s		
NH2+	9.89	vbs	9.91	vbs	9.89	vbs		
4-substituent	S-CH2CH3		S-CH(CH3)2		S-CH2CH2CH3			
	2.89	q(7.4)	3.46	septet(6.8)	2.84	dd(~7.6, ~7.0)		
	1.27	t(7.4)	1.25	d(6.8)	1.64	sextet(7.3)		
					1.02	t(7.3)		
Abbreviations: a – apparent, b – broad, d – doublet, m – multiplet, q – quartet, s – singlet, t – triplet, vbs – very broad singlet								
S.O.E. - 2nd order effects present								

Table IV. Proton NMR Assignments *ortho*-Methoxyphenyl NBOMe Base Compounds.

	25H-NB2OMe base		25D-NB2OMe base		25E-NB2OMe base		25P-NB2OMe base	
position	ppm	peak multiplicity	ppm	peak multiplicity	ppm	peak multiplicity	ppm	peak multiplicity
benzyl 3	6.83	bd(8.6)	6.82	bd(8.6)	6.82	bd(8.6)	6.82	dd(8.4, 1.0)
4	7.21	m	7.21	m	7.21	m	7.21	m
5	6.89	td(7.3, 1.0)	6.89	bt(7.3)	6.88	td(7.6, 1.0)	6.88	td(7.4, 1.0)
6	7.21	m	7.21	m	7.21	m	7.20	m
location of methoxy	2		2		2		2	
OCH3	3.77	s	3.75	s	3.74	s	3.74	s
CH2NHCH2CH2-Ph	3.80	s	3.80	s	3.80	s	3.79	s
CH2NH CH2CH2-Ph	2.83	m	2.82	m	2.83	m	2.82	m
CH2NHCH2 CH2-Ph	2.81	m	2.80	m	2.81	m	2.80	m
Phenyl 3	6.76	d(8.6)	6.66	s	6.67	s	6.66	s
4	6.69	dd(8.6, 3.1)						
6	6.74	d(3.1)	6.65	s	6.66	s	6.65	s
2-OCH3	3.74	s	3.73	s	3.74	s	3.73	s
5-OCH3	3.74	s	3.75	s	3.75	s	3.74	s
4-substituent	H		CH3		CH2-CH3		propyl	
			2.20	s	2.60	q(7.5)	2.70	dd(9.4, 6.0)
					1.18	t(7.5)	1.59	dqd(9.4, 7.4, 6.0)
							0.96	t(7.4)
	25N-NB2OMe base		25C-NB2OMe base		25B-NB2OMe base		25I-NB2OMe base	
benzyl 3	6.84	d(8.3)	6.83	bd(8.2)	6.83	bd(8.1)	6.83	bd(8.4)
4	7.23	t(~8)	7.22	m	7.22	ddd(8.1, 7.4, 1.5)	7.21	m
5	6.90	t(7.7)	6.89	t(7.4, 0.9)	6.89	td(7.4, 1.1)	6.89	t(7.3)
6	7.20	d(~8)	7.20	m	7.19	dd(7.5, 1.5)	7.19	m
location of methoxy	2		2		2		2	
OCH3	3.77	s	3.75	s	3.75	s	3.75	s
CH2NHCH2CH2-Ph	3.79	s	3.79	s	3.78	s	3.79	s
CH2NH CH2CH2-Ph	2.84	m	2.81	m	2.81	m	2.81	m
CH2NHCH2 CH2-Ph	2.88	m	2.79	m	2.78	m	2.78	m
Phenyl 3	7.39	s	6.85	s	7.00	s	7.19	s
4								
6	6.92	s	6.76	s	6.74	s	6.66	s
2-OCH3	3.79	s	3.73	s	3.73	s	3.72	s
5-OCH3	3.89	s	3.82	s	3.81	s	3.79	s
4-substituent	NO2		Cl		Br		I	
	25T2-NB2OMe base		25T4-NB2OMe base		25T7-NB2OMe base			
benzyl 3	6.82	d(~8.3)	6.82	d(7.9)	6.82	bd(~7.6)		
4	7.21	m	7.21	m	7.21	m		
5	6.89	t(~7.5)	6.88	t(~7.3)	6.89	td(7.4, 1.0)		
6	7.20	d(~8)	7.20	m	7.20	m		
location of methoxy	2		2		2			
OCH3	3.75	s	3.75	s	3.75	s		
CH2NHCH2CH2-Ph	3.80	s	3.80	s	3.80	s		
CH2NH CH2CH2-Ph	2.82	m	2.83	m	2.82	m		
CH2NHCH2 CH2-Ph	2.82	m	2.82	m	2.82	m		
Phenyl 3	6.83	s	6.89	s	6.82	s		
4								
6	6.69	s	6.70	s	6.68	s		
2-OCH3	3.75	s	3.74	s	3.74	s		
5-OCH3	3.81	s	3.80	s	3.81	s		
4-substituent	S-CH2CH3		S-CH(CH3)2		S-CH2CH2CH3			
	2.90	q(7.5)	3.45	septet (6.7)	2.85	dd(~7.0, ~7.7)		
	1.29	t(7.5)	1.26	d(6.7)	1.65	sextet(7.3)		
					1.02	t(7.3)		
Abbreviations: a – apparent, b – broad, d – doublet, m – multiplet, q – quartet, s – singlet, t – triplet								

Table V. Proton NMR Assignments *meta*-Methoxyphenyl NBOMe Base Compounds.

	25H-NB3OMe base		25D-NB3OMe base		25E-NB3OMe base		25P-NB3OMe base	
position	ppm	peak multiplicity	ppm	peak multiplicity	ppm	peak multiplicity	ppm	peak multiplicity
benzyl 2	6.75	m	6.93	bs	6.86	bs	6.86	bs
4	6.70	dd(8.8, 3.1)	6.79	dd(8.1, 2.6)	6.78	dd(7.8, 1.6)	6.77	bd(~8.0)
5	7.21	t(~8.0)	7.22	dd(8.1, 7.8)	7.21	t(7.8)	7.21	t(8.0)
6	6.88	m	6.91	d(7.8)	6.87	bd(7.8)	6.87	bd(~8.0)
location of methoxy	3		3		3		3	
OCH3	3.79	s	3.79	s	3.79	s	3.79	s
CH2NHCH2CH2-Ph	3.79	s	3.84	s	3.79	s	3.79	s
CH2NH CH2CH2-Ph	2.87	m	2.91	m	2.87	m	2.87	m
CH2NHCH2 CH2-Ph	2.82	m	2.87	m	2.81	m	2.81	m
Phenyl 3	6.76	m	6.66	s	6.67	s	6.65	s
4	6.78	m						
6	6.86	m	6.67	s	6.68	s	6.67	s
2-OCH3	3.74	s	3.73	s	3.76	s	3.75	s
5-OCH3	3.75	s	3.76	s	3.76	s	3.75	s
4-substituent	H		CH3		CH2-CH3		propyl	
			2.19	s	2.60	q(7.5)	2.54	dd(~8.2, ~7.3)
					1.18	t(7.5)	1.59	m [a-sextet]
							0.95	t(7.3)
	25N-NB3OMe base		25C-NB3OMe base		25B-NB3OMe base		25I-NB3OMe base	
benzyl 2	6.85	d(2.3)	6.85	m	6.89	m	6.84	bs
4	6.79	dd(8.3, 2.3)	6.78	dd(7.8, 2.5)	6.79	ddd(8.3, 2.6, 0.9)	6.78	dd(8.3, 2.6)
5	7.23	dd(8.3, 7.5)[at]	7.22	dd(~8, 7.8)	7.22	t(~8.0)	7.22	at(~8)
6	6.86	bd(7.5)	6.86	m	6.88	m	6.86	d(~8)
location of methoxy	3		3		3		3	
OCH3	3.80	s	3.79	s	3.79	s	3.79	s
CH2NHCH2CH2-Ph	3.80	s	3.78	s	3.81	s	3.78	s
CH2NH CH2CH2-Ph	2.89	m	2.85	m	2.88	m	2.86	m
CH2NHCH2 CH2-Ph	2.86	m	2.81	m	2.82	m	2.79	m
Phenyl 3	7.40	s	6.86	s	7.01	s	7.20	s
4								
6	6.93	s	6.77	s	6.76	s	6.68	s
2-OCH3	3.82	s	3.75	s	3.74	s	3.75	s
5-OCH3	3.90	s	3.83	s	3.82	s	3.80	s
4-substituent	NO2		Cl		Br		I	
	25T2-NB3OMe base		25T4-NB3OMe base		25T7-NB3OMe base			
benzyl 2	6.88	m	6.86	m	6.88	m		
4	6.78	bdd(8.0, 2.6)	6.78	dd(8.1, 2.5)	6.78	dd(8.1, 2.3)		
5	7.22	t(8.0)	7.21	t(8.1)	7.22	t(8.1)		
6	6.88	m	6.86	m	6.88	m		
location of methoxy	3		3		3			
OCH3	3.79	s	3.79	s	3.79	s		
CH2NHCH2CH2-Ph	3.81	s	3.79	s	3.80	s		
CH2NH CH2CH2-Ph	2.88	m	2.87	m	2.87	m		
CH2NHCH2 CH2-Ph	2.83	m	2.81	m	2.83	m		
Phenyl 3	6.83	s	6.90	s	6.83	s		
4								
6	6.70	s	6.71	s	6.69	s		
2-OCH3	3.76	s	3.76	s	3.76	s		
5-OCH3	3.82	s	3.81	s	3.82	s		
4-substituent	S-CH2CH3		S-CH(CH3)2		S-CH2CH2CH3			
	2.90	q(7.5)	3.45	septet(6.7)	2.85	m		
	1.29	t(7.5)	1.26	d(6.7)	1.65	sextet(7.4)		
					1.02	t(7.4)		
Abbreviations: a – apparent, b – broad, d – doublet, m – multiplet, q – quartet, s – singlet, t – triplet								

Table VI. Proton NMR Assignments *para*-Methoxyphenyl NBOMe Base Compounds.

	25H-NB4OMe base		25D-NB4OMe base		25E-NB4OMe base		25P-NB4OMe base	
	ppm	peak multiplicity	ppm	peak multiplicity	ppm	peak multiplicity	ppm	peak multiplicity
benzyl 2	7.21	d(8.7)	7.21	d(8.7)	7.21	d(8.5)	7.21	d(8.8)
3	6.84	d(8.7)	6.84	d(8.7)	6.84	d(8.5)	6.84	d(8.8)
5	6.84	d(8.7)	6.84	d(8.7)	6.84	d(8.5)	6.84	d(8.8)
6	7.21	d(8.7)	7.21	d(8.7)	7.21	d(8.5)	7.21	d(8.8)
location of methoxy	4		4		4		4	
OCH3	3.79	s	3.79	s	3.79	s	3.79	s
CH2NHCH2CH2-Ph	3.74	s	3.79	s	3.75	s	3.75	s
CH2NH CH2CH2-Ph	2.86	m	2.86	m	2.86	m	2.86	m
CH2NHCH2 CH2-Ph	2.81	m	2.80	m	2.80	m	2.81	m
Phenyl 3	6.76	d(8.7)	6.65	s	6.67	s	6.66	s
4	6.70	dd(8.7, 3.0)						
6	6.74	d(3.0)	6.66	s	6.68	s	6.67	s
2-OCH3	3.75	s	3.75	s	3.76	s	3.75	s
5-OCH3	3.76	s	3.76	s	3.76	s	3.75	s
4-substituent	H		CH3		CH2CH3		propyl	
			2.20	s	2.60	q(7.5)	2.54	dd(~8,~7)
					1.18	t(7.5)	1.60	m
							0.95	t(7.3)
	25N-NB4OMe base		25C-NB4OMe base		25B-NB4OMe base		25I-NB4OMe base (600 MHz)	
	ppm	peak multiplicity	ppm	peak multiplicity	ppm	peak multiplicity	ppm	peak multiplicity
benzyl 2	7.20	d(8.4)	7.20	d(8.5)	7.20	d(8.5)	7.20	d(8.3)
3	6.85	d(8.4)	6.85	d(8.5)	6.84	d(8.5)	6.84	d(8.3)
5	6.85	d(8.4)	6.85	d(8.5)	6.84	d(8.5)	6.84	d(8.3)
6	7.20	d(8.4)	7.20	d(8.5)	7.20	d(8.5)	7.20	d(8.3)
location of methoxy	4		4		4		4	
OCH3	3.80	s	3.79	s	3.79	s	3.79	s
CH2NHCH2CH2-Ph	3.75	s	3.74	s	3.73	s	3.73	s
CH2NH CH2CH2-Ph	2.87	abs	2.84	m	2.84	m	2.84	m
CH2NHCH2 CH2-Ph	2.87	abs	2.79	m	2.78	m	2.78	m
Phenyl 3	7.40	s	6.87	s	7.01	s	7.20	s
4								
6	6.93	s	6.77	s	6.75	s	6.67	s
2-OCH3	3.82	s	3.75	s	3.75	s	3.75	s
5-OCH3	3.90	s	3.83	s	3.82	s	3.80	s
4-substituent	NO2		Cl		Br		I	
	25T2-NB4OMe base		25T4-NB4OMe base		25T7-NB4OMe base			
	ppm	peak multiplicity	ppm	peak multiplicity	ppm	peak multiplicity	ppm	peak multiplicity
benzyl 2	7.20	d(8.6)	7.20	d(8.6)	7.23	d(8.7)		
3	6.84	d(8.6)	6.84	d(8.6)	6.85	d(8.7)		
5	6.84	d(8.6)	6.84	d(8.6)	6.85	d(8.7)		
6	7.20	d(8.6)	7.20	d(8.6)	7.23	d(8.7)		
location of methoxy	4		4		4			
OCH3	3.79	s	3.79	s	3.78	s		
CH2NHCH2CH2-Ph	3.74	s	3.75	s	3.77	s		
CH2NH CH2CH2-Ph	2.85	m	2.86	m	2.86	m		
CH2NHCH2 CH2-Ph	2.80	m	2.81	m	2.84	m		
Phenyl 3	6.84	s	6.90	s	6.82	s		
4								
6	6.69	s	6.70	s	6.69	s		
2-OCH3	3.77	s	3.76	s	3.76	s		
5-OCH3	3.82	s	3.81	s	3.82	s		
4-substituent	S-CH2CH3		S-CH(CH3)2		S-CH2CH2CH3			
	2.90	q(7.4)	3.46	septet(6.7)	2.85	m		
	1.29	t(7.4)	1.26	d(6.7)	1.65	sextet(7.3)		
					1.02	t(7.3)		
Abbreviations: a – apparent, b – broad, d – doublet, m – multiplet, q – quartet, s – singlet, t – triplet								

Table VII. Carbon-13 NMR Assignments *ortho*-Methoxyphenyl NBOMe HCl Compounds.

position	25H- NB2OMe HCl	25D- NB2OMe HCl	25E- NB2OMe HCl	25P- NB2OMe HCl	25N- NB2OMe HCl	25C- NB2OMe HCl	25B- NB2OMe HCl	25I- NB2OMe HCl	25T2- NB2OMe HCl	25T4- NB2OMe HCl	25T7- NB2OMe HCl
benzyl 1	118.6	118.5	118.6	118.5	118.3	118.3	118.4	118.4	118.5	118.5	118.5
2	157.7	157.6	157.6	157.6	157.9	157.6	157.6	157.7	157.7	157.7	157.7
3	110.4	110.4	110.4	110.3	110.5	110.5	110.2	110.4	110.4	110.5	110.4
4	131.1	131.1	131.0	131.0	131.2	131.2	131.1	131.1	131.1	131.1	131.1
5	121.0	121.1	121.0	121.0	120.9	121.1	121.0	120.9	120.9	121.0	121.0
6	132.1	132.0	132.0	132.0	132.0	132.0	132.0	132.0	132.1	132.0	132.0
location of methoxy	2	2	2	2	2	2	2	2	2	2	2
OCH ₃	55.4	55.3	55.4	55.3	55.5	55.4	55.4	55.5	55.5	55.5	55.4
CH ₂ NHCH ₂ CH ₂ -Ph	46.7	47.0	46.7	46.7	46.1	46.9	46.7	45.8	46.4	46.5	46.6
CH ₂ NH CH ₂ CH ₂ -Ph	45.4	45.6	45.6	45.6	44.7	45.1	45.0	45.0	45.3	45.3	45.4
CH ₂ NHCH ₂ CH ₂ -Ph	28.0	28.0	27.9	27.9	28.0	27.9	27.9	28.0	27.8	27.8	27.8
phenyl 1	125.8	122.1	122.3	122.3	132.7	123.9	124.8	126.0	123.5	124.6	123.2
2	151.6	151.0	151.2	151.0	150.5	151.4	151.6	152.0	151.4	151.1	151.4
3	111.5	113.8	112.2	112.9	107.5	113.1	115.9	121.6	113.1	115.9	113.0
4	113.2	126.4	132.5	131.0	137.9	121.4	110.4	83.8	123.8	122.7	124.2
5	153.7	151.7	151.3	151.4	147.6	149.2	150.1	152.6	151.8	152.9	151.8
6	116.8	113.6	113.9	113.9	117.3	115.6	115.4	114.1	114.0	114.2	114.0
2-OCH ₃	55.8	55.8	55.8	55.7	56.0	55.9	55.9	55.9	55.9	55.9	55.9
5-OCH ₃	55.7	56.2	56.2	56.2	57.4	57.0	57.1	57.2	56.6	56.6	56.6
4-substituent	H	CH ₃	CH ₂ -CH ₃	propyl	NO ₂	Cl	Br	I	S-CH ₂ - CH ₃	S-CH- (CH ₃) ₂	S-CH ₂ - CH ₂ -CH ₃
		16.3	23.4	32.4					26.7	36.7	34.6
			14.4	23.2					14.2	23.1	22.5
				14.1							13.5
Notes:	600 MHz										

Table VIII. Carbon-13 NMR Assignments *meta*-Methoxyphenyl NBOMe HCl Compounds.

position	25H- NB3OMe HCl	25D- NB3OMe HCl	25E- NB3OMe HCl	25P- NB3OMe HCl	25N- NB3OMe HCl	25C- NB3OMe HCl	25B- NB3OMe HCl	25I- NB3OMe HCl	25T2- NB3OMe HCl	25T4- NB3OMe HCl	25T7- NB3OMe HCl
benzyl 1	131.6	131.6	132.4	131.7	131.2	131.4	131.4	131.4	131.5	131.5	131.5
2	115.1	115.1	115.1	115.1	115.5	115.3	115.2	115.2	115.3	115.3	115.2
3	160.0	160.0	160.0	160.0	160.0	160.0	160.0	160.0	160.0	160.0	160.0
4	115.7	115.6	115.6	115.6	115.4	115.5	115.5	115.6	115.5	115.5	115.6
5	130.0	130.0	130.0	130.0	130.1	130.0	130.0	130.0	130.0	130.0	130.0
6	122.4	122.3	122.3	122.4	122.3	122.3	122.3	122.4	122.4	122.4	122.4
location of methoxy	3	3	3	3	3	3	3	3	3	3	3
OCH ₃	55.5	55.5	55.5	55.5	55.4	55.4	55.4	55.5	55.5	55.5	55.5
CH ₂ NHCH ₂ CH ₂ -Ph	50.4	50.5	50.5	50.5	50.7	50.6	50.6	50.6	50.5	50.5	50.5
CH ₂ NH CH ₂ CH ₂ -Ph	45.1	45.4	45.3	45.3	44.7	45.0	44.9	44.9	45.2	45.1	45.2
CH ₂ NHCH ₂ CH ₂ -Ph	27.9	27.8	27.8	27.8	28.0	27.7	27.8	28.0	27.8	27.8	27.8
phenyl 1	125.8	122.4	122.4	122.4	132.4	124.0	124.8	126.0	123.4	124.6	123.3
2	151.6	151.0	151.2	151.1	150.6	151.4	151.7	152.1	151.4	151.2	151.4
3	111.3	113.7	112.0	112.8	107.6	113.0	115.8	121.6	113.1	116.0	113.0
4	113.0	126.3	131.6	130.9	138.0	121.3	110.2	83.9	123.8	122.7	124.1
5	153.5	151.6	151.2	151.4	147.6	149.0	150.0	152.6	151.8	152.9	151.8
6	116.7	113.4	113.7	113.8	117.2	115.5	115.2	114.0	113.9	114.0	113.9
2-OCH ₃	55.6	55.7	55.7	55.7	56.0	55.8	55.9	55.9	55.9	55.8	55.9
5-OCH ₃	55.8	56.1	56.2	56.2	57.3	56.9	57.0	57.2	56.6	56.6	56.6
4-substituent	H	CH ₃	CH ₂ -CH ₃	propyl	NO ₂	Cl	Br	I	S-CH ₂ - CH ₃	S-CH- (CH ₃) ₂	S-CH ₂ - CH ₂ -CH ₃
		16.2	23.4	32.4					26.7	36.7	34.6
			14.3	23.2					14.2	23.1	22.5
				14.1							13.5

Table IX. Carbon-13 NMR Assignments *para*-Methoxyphenyl NBOMe HCl Compounds.

position	25H- NB4OMe HCl	25D- NB4OMe HCl	25E- NB4OMe HCl	25P- NB4OMe HCl	25N- NB4OMe HCl	25C- NB4OMe HCl	25B- NB4OMe HCl	25I- NB4OMe HCl	25T2- NB4OMe HCl	25T4- NB4OMe HCl	25T7- NB4OMe HCl
benzyl 1	122.1	122.2	122.2	122.2	121.8	121.9	121.9	122.0	122.1	122.6	122.1
2	131.9	131.9	131.9	131.9	131.9	131.9	131.9	131.9	131.9	131.9	131.9
3	114.3	114.3	114.3	114.3	114.4	114.3	114.3	114.3	114.3	114.3	114.3
4	160.3	160.3	160.3	160.3	160.5	160.3	160.3	160.4	160.3	160.3	160.3
5	114.3	114.3	114.3	114.3	114.4	114.3	114.3	114.3	114.3	114.3	114.3
6	131.9	131.9	131.9	131.9	131.9	131.9	131.9	131.9	131.9	131.9	131.9
location of methoxy	4	4	4	4	4	4	4	4	4	4	4
OCH ₃	55.7	55.1	55.1	55.1	55.1	55.1	55.1	55.1	55.1	55.1	55.1
CH ₂ NHCH ₂ CH ₂ -Ph	50.0	50.1	50.1	50.1	50.5	50.2	50.2	50.2	50.1	50.1	50.1
CH ₂ NH CH ₂ CH ₂ -Ph	45.1	45.4	45.4	45.4	44.7	45.0	44.9	45.0	45.2	45.1	45.2
CH ₂ NHCH ₂ CH ₂ -Ph	27.8	27.8	27.8	27.8	28.0	27.7	27.8	28.0	27.7	27.8	27.7
phenyl 1	125.9	122.5	122.5	122.6	132.4	124.2	124.9	126.1	123.6	124.8	123.5
2	151.6	151.0	151.3	151.1	150.6	151.4	151.7	152.1	151.4	151.2	151.4
3	111.3	113.7	112.1	112.9	107.6	113.0	115.8	121.6	113.1	116.0	113.0
4	113.0	126.2	132.4	130.9	138.1	121.3	110.1	83.8	123.7	122.1	124.0
5	153.6	151.6	151.3	151.4	147.6	149.0	150.1	152.6	151.8	152.9	151.8
6	116.6	113.4	113.7	113.8	117.1	115.4	115.2	114.0	113.9	114.0	113.9
2-OCH ₃	55.2	55.8	55.8	55.8	56.1	55.9	55.9	56.0	55.9	55.9	55.9
5-OCH ₃	55.8	56.1	56.2	56.2	57.4	56.9	57.0	57.2	56.6	56.6	56.6
4-substituent	H	CH ₃	CH ₂ -CH ₃	propyl	NO ₂	Cl	Br	I	S-CH ₂ - CH ₃	S-CH- (CH ₃) ₂	S-CH ₂ - CH ₂ -CH ₃
		16.2	23.4	32.4					26.7	36.7	34.6
			14.4	23.2					14.2	23.1	22.5
				14.1							13.5

Table X. Carbon-13 NMR Assignments *ortho*-Methoxyphenyl NBOMe Base Compounds.

	25H- NB2OMe base	25D- NB2OMe base	25E- NB2OMe base	25P- NB2OMe base	25N- NB2OMe base	25C- NB2OMe base	25B- NB2OMe base	25I- NB2OMe base	25T2- NB2OMe base	25T4- NB2OMe base	25T7- NB2OMe base
benzyl 1	128.4	128.5	128.5	129.8	129.8	128.1	128.3	129.8	128.3	128.3	128.4
2	157.6	157.6	157.6	157.6	157.6	157.6	157.6	157.6	157.6	157.6	157.6
3	110.1	110.1	110.1	110.1	110.2	110.1	110.2	110.1	110.1	110.2	110.2
4	128.0	128.0	128.0	128.0	128.1	128.1	128.2	128.1	128.1	128.1	128.1
5	120.3	120.3	120.3	120.3	120.4	119.9	120.3	120.3	120.3	120.3	120.3
6	129.8	129.7	129.8	129.6	128.3	129.8	129.9	128.3	129.8	129.8	129.8
location of methoxy	2	2	2	2	2	2	2	2	2	2	2
OCH3	55.1	55.1	55.1	55.1	55.2	55.1	55.1	55.2	55.1	55.1	55.1
CH2NHCH2CH2-Ph	49.1	49.1	49.1	49.1	49.2	49.2	49.1	49.2	49.1	49.2	49.2
CH2NH CH2 CH2-Ph	48.8	49.2	49.2	49.0	48.1	48.6	48.4	48.5	48.7	48.8	48.9
CH2NHCH2 CH2-Ph	30.9	30.8	30.8	30.8	31.3	30.8	30.9	31.1	30.8	30.9	30.9
phenyl 1	129.9	126.4	126.4	126.4	137.1	128.3	128.9	130.1	127.9	128.9	127.8
2	151.9	151.4	151.1	151.3	150.9	151.8	152.1	152.4	151.7	151.5	151.8
3	111.3	114.0	112.4	113.5	107.4	113.0	115.9	121.6	114.1	116.7	114.0
4	111.2	124.8	131.1	129.8	137.1	120.3	108.8	82.3	121.8	120.8	122.2
5	153.4	151.5	151.6	151.4	147.6	148.8	149.8	152.5	152.0	153.0	152.0
6	116.6	113.2	113.4	113.2	116.2	115.1	114.9	113.7	113.6	113.7	113.7
2-OCH3	55.9	56.1	56.1	56.1	56.0	56.0	56.1	56.1	56.2	56.1	56.2
5-OCH3	55.6	56.1	56.2	56.1	57.1	56.9	57.0	57.1	56.4	56.4	56.5
4-substituent	H	CH3	CH2-CH3	propyl	NO2	Cl	Br	I	S- CH2CH3	S-CH- (CH3)2	S-CH2- CH2-CH3
		16.1	23.3	32.3					27.0	36.9	35.0
			14.5	23.3					14.3	23.1	22.6
				14.1							13.5
Notes:							600 MHz				

Table XI. Carbon-13 NMR Assignments *meta*-Methoxyphenyl NBOMe Base Compounds.

	25H- NB3OMe base	25D- NB3OMe base	25E- NB3OMe base	25P- NB3OMe base	25N- NB3OMe base	25C- NB3OMe base	25B- NB3OMe base	25I- NB3OMe base	25T2- NB3OMe base	25T4- NB3OMe base	25T7- NB3OMe base
benzyl 1	142.2	140.3	142.2	142.2	141.9	142.0	140.9	142.1	141.3	142.1	141.2
2	116.7	113.8	113.5	113.5	113.7	113.5	113.7	113.6	113.7	113.6	113.7
3	159.7	159.8	159.7	159.7	159.8	159.7	159.8	159.8	159.8	159.8	159.8
4	111.3	113.1	112.4	112.4	112.3	112.3	112.7	112.4	112.6	112.4	112.6
5	129.3	129.4	129.3	129.3	129.4	129.3	129.4	129.3	129.4	128.8	129.4
6	120.4	120.8	120.4	120.4	120.4	120.1	120.5	120.4	120.5	120.4	120.5
location of methoxy	3	3	3	3	3	3	3	3	3	3	3
OCH3	55.2	55.2	55.2	55.2	55.2	55.2	55.2	55.2	55.2	55.2	55.2
CH2NHCH2CH2-Ph	53.7	53.1	53.7	53.7	53.7	53.7	53.4	53.7	53.5	53.7	53.5
CH2NH CH2 CH2-Ph	49.1	48.6	49.4	49.3	48.4	48.9	48.4	48.9	48.9	49.1	48.9
CH2NHCH2 CH2-Ph	30.9	30.2	30.8	30.8	31.3	30.8	30.6	31.1	30.6	31.0	30.6
phenyl 1	129.7	125.4	126.2	126.2	136.9	128.0	128.3	129.9	127.4	129.3	127.3
2	151.9	151.3	151.2	151.3	150.9	151.8	152.0	152.5	151.7	151.5	151.7
3	111.4	113.9	113.4	113.2	107.5	113.1	115.9	121.7	114.0	116.7	113.9
4	112.4	125.3	131.2	129.7	137.2	120.3	109.0	82.4	122.2	121.0	122.5
5	153.4	151.5	151.6	151.4	147.7	148.9	149.9	152.5	152.0	153.0	152.0
6	113.4	113.2	112.4	113.4	116.3	115.1	114.9	113.7	113.6	113.7	113.7
2-OCH3	55.7	56.0	56.1	56.1	56.1	56.0	56.1	56.1	56.2	56.4	56.2
5-OCH3	55.9	56.1	56.2	56.2	57.1	56.9	57.0	57.1	56.5	56.1	56.5
4-substituent	H	CH3	CH2-CH3	propyl	NO2	Cl	Br	I	S- CH2CH3	S-CH- (CH3)2	S-CH2- CH2-CH3
		16.2	23.3	32.3					27.0	36.9	34.9
			14.5	23.3					14.3	23.1	22.6
				14.1							13.6

Table XII. Carbon-13 NMR Assignments *para*-Methoxyphenyl NBOMe Base Compounds.

	25H- NB4OMe base	25D-NB4OMe base	25E- NB4OMe base	25P- NB4OMe base	25N- NB4OMe base	25C- NB4OMe base	25B- NB4OMe base	25I- NB4OMe base	25T2- NB4OMe base	25T4- NB4OMe base	25T7- NB4OMe base
benzyl 1	132.6	129.1 or 130.0	129.1	132.6	132.3	132.5	132.4	131.0	132.5	132.6	131.4
2	129.3	130.0	129.9	129.3	129.3	129.2	129.3	129.6	129.3	129.3	129.6
3	113.7	113.9	113.9	113.7	113.8	113.7	113.8	113.8	113.8	113.8	113.9
4	158.5	159.0	159.0	158.6	158.7	158.6	158.6	158.9	158.6	158.6	158.8
5	113.7	113.9	113.9	113.7	113.8	113.7	113.8	113.8	113.8	113.8	113.9
6	129.3	130.0	129.9	129.3	129.3	129.2	129.3	129.6	129.3	129.3	129.6
location of methoxy	4	4	4	4	4	4	4	4	4	4	4
OCH3	55.3	55.2	55.2	55.3	55.3	55.2	55.3	55.3	55.3	55.3	55.3
CH2NHCH2CH2-Ph	53.1	52.4	52.5	53.2	53.2	53.1	53.1	52.8	53.2	53.2	52.8
CH2NHCH2CH2-Ph	49.0	48.4	48.4	49.3	48.3	48.9	48.7	48.4	49.1	49.0	48.7
CH2NHCH2CH2-Ph	30.9	30.0	30.1	30.8	31.3	30.8	30.9	30.7	30.8	31.0	30.5
phenyl 1	129.7	125.3	125.3	126.2	137.0	128.0	128.8	129.4	127.7	128.8	127.1
2	151.9	151.2	151.5	151.3	150.9	151.8	152.1	152.4	151.7	151.5	151.7
3	111.4	113.9	112.3	113.2	107.5	113.1	115.9	121.7	114.1	116.7	113.8
4	111.3	125.2	131.5	129.7	137.2	120.1	108.9	82.6	122.1	120.9	122.6
5	153.4	151.6	151.2	151.4	147.7	148.9	149.9	152.5	152.0	153.0	152.0
6	116.7	113.2	113.5	113.5	116.3	115.1	114.9	113.7	113.6	113.7	113.7
2-OCH3	55.7	56.0	56.1	56.1	56.1	56.0	56.1	56.1	56.2	56.1	56.2
5-OCH3	55.9	56.1	56.2	56.2	57.1	56.9	57.0	57.1	56.5	56.4	56.5
4-substituent	H	CH3	CH2CH3	propyl	NO2	Cl	Br	I	S- CH2CH3	S-CH- (CH3)2	S-CH2- CH2-CH3
		16.2	23.3	32.3					27.0	36.9	34.9
			14.4	23.3					14.3	23.1	22.5
				14.1							13.6
Notes:			600 MHz					600 MHz			

-END-